Linear discriminant functions

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Machine Learning

Discriminative learning

Discriminative vs generative

- Generative learning assumes knowledge of the distribution governing the data
- Discriminative learning focuses on directly modeling the discriminant function
- E.g. for classification, directly modeling decision boundaries (rather than inferring them from the modelled data distributions)

Discriminative learning

PROS

- When data are complex, modeling their distribution can be very difficult
- If data discrimination is the goal, data distribution modeling is not needed
- Focuses parameters (and thus use of available training examples) on the desired goal

CONS

- The learned model is less flexible in its usage
- It does not allow to perform arbitrary inference tasks
- E.g. it is not possible to efficiently generate new data from a certain class

Linear discriminant functions

Description

$$f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0$$

- The discriminant function is a linear combination of example features
- w_0 is called *bias* or *threshold*
- it is the simplest possible discriminant function
- Depending on the complexity of the task and amount of data, it can be the best option available (at least it is the first to try)

Linear binary classifier

Description

$$f(\boldsymbol{x}) = \mathrm{sign}(\boldsymbol{w}^T \boldsymbol{x} + w_0)$$

- It is obtained taking the sign of the linear function
- The decision boundary ($f(\mathbf{x}) = 0$) is a hyperplane (H)
- The weight vector $\boldsymbol{w}$ is orthogonal to the decision hyperplane:

$$\forall \boldsymbol{x}, \boldsymbol{x}' : f(\boldsymbol{x}) = f(\boldsymbol{x}') = 0$$
$$\boldsymbol{w}^T \boldsymbol{x} + w_0 - \boldsymbol{w}^T \boldsymbol{x}' - w_0 = 0$$
$$\boldsymbol{w}^T (\boldsymbol{x} - \boldsymbol{x}') = 0$$

Linear binary classifier

Functional margin

- The value $f(\boldsymbol{x})$ of the function for a certain point $\boldsymbol{x}$ is called *functional margin*
- It can be seen as a confidence in the prediction

Geometric margin

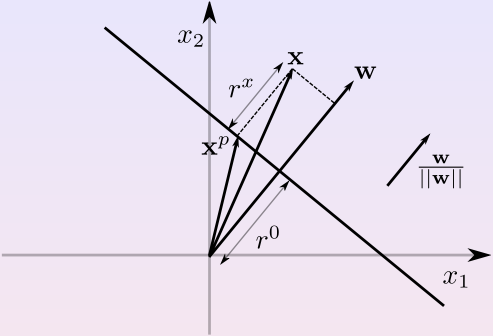
- The distance from $\boldsymbol{x}$ to the hyperplane is called *geometric margin*

$$r^x = \frac{f(\boldsymbol{x})}{||\boldsymbol{w}||}$$

- It is a normalize version of the functional margin
- The distance from the origin to the hyperplane is:

$$r^0 = \frac{f(\mathbf{0})}{||\boldsymbol{w}||} = \frac{w_0}{||\boldsymbol{w}||}$$

Linear binary classifier



Geometric margin (cont)

- A point can be expressed by its projection on H plus its distance to H times the unit vector in that direction:

$$\boldsymbol{x} = \boldsymbol{x}^p + r^x \frac{\boldsymbol{w}}{||\boldsymbol{w}||}$$

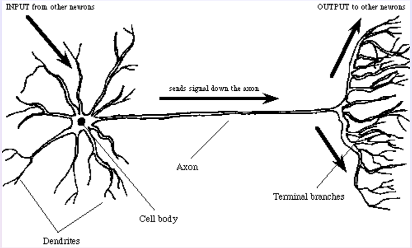
Linear binary classifier

Geometric margin (cont)

- Then as $f(\boldsymbol{x}^p) = 0$:

$$\begin{aligned}
f(\boldsymbol{x}) &= \boldsymbol{w}^T\boldsymbol{x} + w_0 \\
&= \boldsymbol{w}^T(\boldsymbol{x}^p + r^x\frac{\boldsymbol{w}}{||\boldsymbol{w}||}) + w_0 \\
&= \underbrace{\boldsymbol{w}^T\boldsymbol{x}^p + w_0}_{f(\boldsymbol{x}^p)} + r^x\boldsymbol{w}^T\frac{\boldsymbol{w}}{||\boldsymbol{w}||} \\
&= r^x||\boldsymbol{w}|| \\
\frac{f(\boldsymbol{x})}{||\boldsymbol{w}||} &= r^x
\end{aligned}$$

Biological motivation

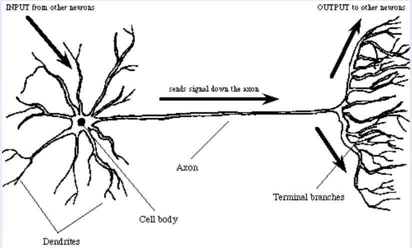


Human Brain

- Composed of densely interconnected network of **neurons**
- A neuron is made of:

soma	A central body containing the nucleus
dendrites	A set of filaments departing from the body
axon	a longer filament (up to 100 times body diameter)
synapses	connections between dendrites and axons from other neurons

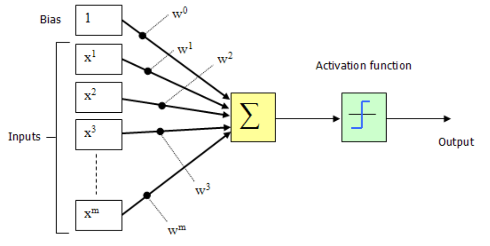
Biological motivation



Human Brain

- Electrochemical reactions allow signals to propagate along neurons via axons, synapses and dendrites
- Synapses can either *excite* on *inhibit* a neuron potentional
- Once a neuron potential exceeds a certain *threshold*, a signal is generated and transmitted along the axon

Perceptron



Single neuron architecture

$$f(x) = \mathrm{sign}(\boldsymbol{w}^T \boldsymbol{x} + w_0)$$

- Linear combination of input features
- Threshold activation function

Perceptron

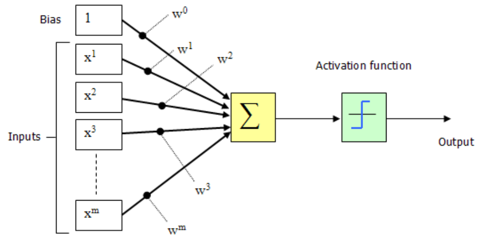
Representational power

- *Linearly separable* sets of examples
- E.g. primitive boolean functions (AND,OR,NAND,NOT)
- $\Rightarrow$ any logic formula can be represented by a network of two levels of perceptrons (in disjunctive or conjunctive normal form).

Problem

- *non-linearly separable* sets of examples cannot be separated
- Representing complex logic formulas can require a number of perceptrons *exponential* in the size of the input

Perceptron



Augmented feature/weight vectors

$$f(x) = \text{sign}(\hat{\boldsymbol{w}}^T \hat{\boldsymbol{x}})$$

- Where bias is incorporated in augmented vectors:

$$\hat{\boldsymbol{w}} = \begin{pmatrix} w_0 \\ \boldsymbol{w} \end{pmatrix} \qquad \hat{\boldsymbol{x}} = \begin{pmatrix} 1 \\ \boldsymbol{x} \end{pmatrix}$$

- Search for weight vector + bias is replaced by search for augmented weight vector (we skip the "^" in the following)

Parameter learning

Error minimization

- Need to find a function of the parameters to be optimized (like in maximum likelihood for probability distributions)
- Reasonable function is measure of error on training set $\mathcal{D}$ (i.e. the loss ℓ):

$$E(\boldsymbol{w}; \mathcal{D}) = \sum_{(\boldsymbol{x}, y) \in \mathcal{D}} \ell(y, f(\boldsymbol{x}))$$

- Problem of overfitting training data (less severe for linear classifier, we will discuss it)

Parameter learning

Gradient descent

1. Initialize $\boldsymbol{w}$ (e.g. $\boldsymbol{w} = 0$)
2. Iterate until gradient is approx. zero:

$$\boldsymbol{w} = \boldsymbol{w} - \eta \nabla E(\boldsymbol{w}; \mathcal{D})$$

Note

- η is called *learning rate* and controls the amount of movement at each gradient step
- The algorithm is guaranteed to converge to a local optimum of $E(\boldsymbol{w}; \mathcal{D})$ (for small enough η)
- Too low η implies slow convergence
- Techniques exist to adaptively modify η

Parameter learning

Problem

- The misclassification loss is piecewise constant
- Poor candidate for gradient descent

Perceptron training rule

$$E(\boldsymbol{w};\mathcal{D}) = \sum_{(\boldsymbol{x},y)\in\mathcal{D}_E} -yf(\boldsymbol{x})$$

- $\mathcal{D}_E$ is the set of current training errors for which:

$$yf(\boldsymbol{x}) \leq 0$$

- The error is the sum of the functional margins of incorrectly classified examples

Parameter learning

Perceptron training rule

- The error gradient is:

$$\begin{aligned} \nabla E(\mathbf{w};\mathcal{D}) &= \nabla \sum_{(\mathbf{x},y)\in\mathcal{D}_E} -yf(\mathbf{x}) \\ &= \nabla \sum_{(\mathbf{x},y)\in\mathcal{D}_E} -y(\mathbf{w}^T\mathbf{x}) \\ &= \sum_{(\mathbf{x},y)\in\mathcal{D}_E} -y\mathbf{x} \end{aligned}$$

- the amount of update is:

$$-\eta\nabla E(\mathbf{w};\mathcal{D}) = \eta \sum_{(\mathbf{x},y)\in\mathcal{D}_E} y\mathbf{x}$$

Perceptron learning

Stochastic perceptron training rule

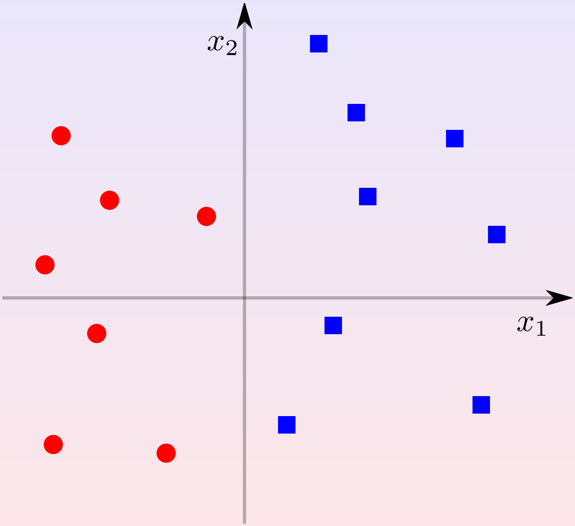
1. Initialize weights randomly
2. Iterate until all examples correctly classified:
    1. For each incorrectly classified training example $(\boldsymbol{x}, y)$ update weight vector:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta y \mathbf{x}$$

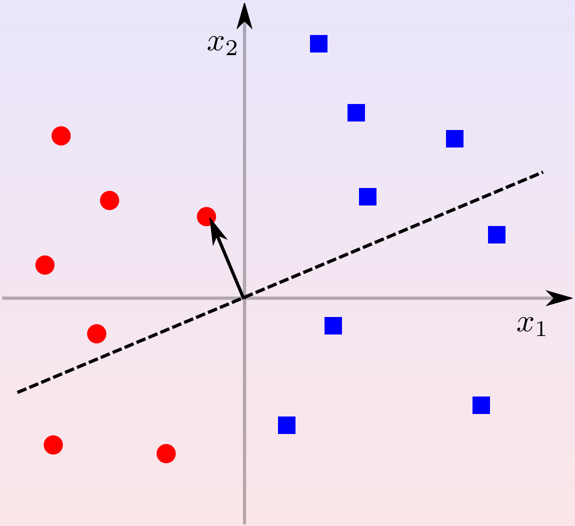
Note on stochastic

- we make a gradient step for each training error (rather than on the sum of them in *batch* learning)
- Each gradient step is very fast
- Stochasticity can sometimes help to avoid local minima, being guided by various gradients for each training example (which won't have the same local minima in general)

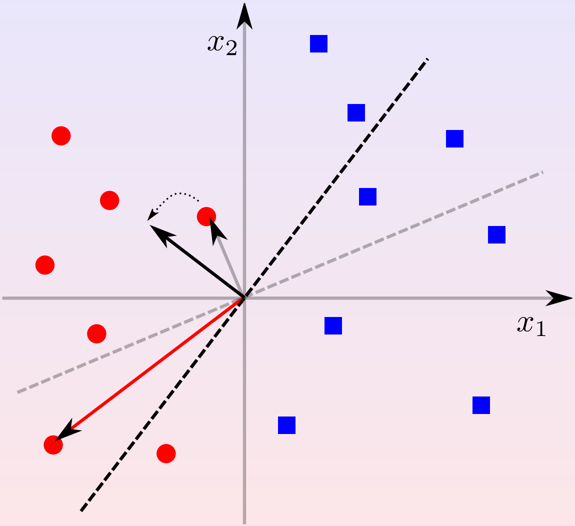
Perceptron learning



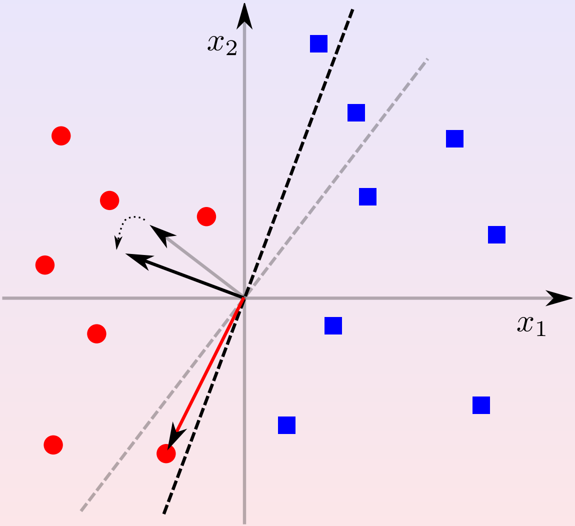
Perceptron learning



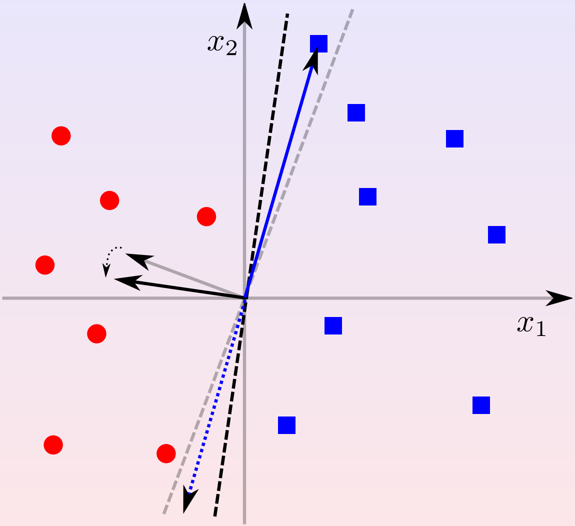
Perceptron learning



Perceptron learning



Perceptron learning



Perceptron regression

Exact solution

- Let $X \in \mathbb{R}^n \times \mathbb{R}^d$ be the input training matrix (i.e. $X = [\boldsymbol{x}^1 \cdots \boldsymbol{x}^n]^T$ for $n = |\mathcal{D}|$ and $d = |\boldsymbol{x}|$)
- Let $\boldsymbol{y} \in \mathbb{R}^n$ be the output training matrix (i.e. y_i is output for example $\mathbf{x}^i$)
- Regression learning could be stated as a set of linear equations):

$$X\boldsymbol{w} = \boldsymbol{y}$$

- Giving as solution:

$$\boldsymbol{w} = X^{-1}\boldsymbol{y}$$

Perceptron regression

Problem

- Matrix X is rectangular, usually more rows than columns
- System of equations is overdetermined (more equations than unknowns)
- No exact solution typically exists

Perceptron regression

Mean squared error (MSE)

- Resort to loss minimization
- Standard loss for regression is the mean squared error:

$$E(\boldsymbol{w};\mathcal{D}) = \sum_{(\boldsymbol{x},y)\in\mathcal{D}} (y - f(\boldsymbol{x}))^2 = (\boldsymbol{y} - X\boldsymbol{w})^T(\boldsymbol{y} - X\boldsymbol{w})$$

- Closed form solution exists
- Can always be solved by gradient descent (can be faster)
- Can also be used as a classification loss

Perceptron regression

Closed form solution

$$
\begin{aligned}
\nabla E(\boldsymbol{w}; \mathcal{D}) &= \nabla (\boldsymbol{y} - X\boldsymbol{w})^T (\boldsymbol{y} - X\boldsymbol{w}) \\
&= 2(\boldsymbol{y} - X\boldsymbol{w})^T (-X) = 0 \\
&= -2\boldsymbol{y}^T X + 2\boldsymbol{w}^T X^T X = 0 \\
\boldsymbol{w}^T X^T X &= \boldsymbol{y}^T X \\
X^T X \boldsymbol{w} &= X^T \boldsymbol{y} \\
\boldsymbol{w} &= (X^T X)^{-1} X^T \boldsymbol{y}
\end{aligned}
$$

Perceptron regression

$$\boldsymbol{w} = (X^T X)^{-1} X^T \boldsymbol{y}$$

Note

- $(X^T X)^{-1} X^T$ is called *left-inverse*
- If X is square and nonsingular, inverse and left-inverse coincide and the MSE solution corresponds to the exact one
- The left-inverse exists provided $(X^T X) \in \mathbb{R}^{d \times d}$ is full rank $\rightarrow$ features are linearly independent (if not, just remove the redundant ones!)

Perceptron regression

Gradient descent

$$\begin{aligned}
\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i}\frac{1}{2}\sum_{(\boldsymbol{x},y)\in\mathcal{D}}(y - f(\boldsymbol{x}))^2 \\
&= \frac{1}{2}\sum_{(\boldsymbol{x},y)\in\mathcal{D}}\frac{\partial}{\partial w_i}(y - f(\boldsymbol{x}))^2 \\
&= \frac{1}{2}\sum_{(\boldsymbol{x},y)\in\mathcal{D}}2(y - f(\boldsymbol{x}))\frac{\partial}{\partial w_i}(y - \boldsymbol{w}^T\boldsymbol{x}) \\
&= \sum_{(\boldsymbol{x},y)\in\mathcal{D}}(y - f(\boldsymbol{x}))(-x_i)
\end{aligned}$$

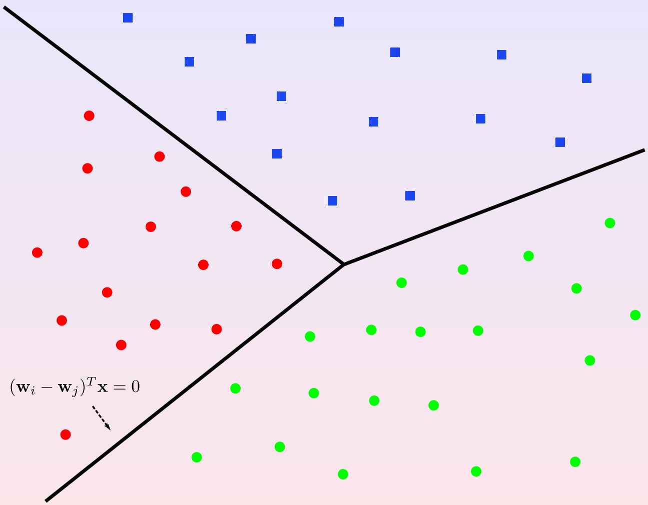
Multiclass classification

One-vs-all

- Learn one binary classifier for each class:
  - positive examples are examples of the class
  - negative examples are examples of all other classes
- Predict a new example in the class with maximum functional margin
- Decision boundaries for which $f_i(\boldsymbol{x}) = f_j(\boldsymbol{x})$ are pieces of hyperplanes:

$$\begin{aligned} \boldsymbol{w}_i^T \boldsymbol{x} &= \boldsymbol{w}_j^T \boldsymbol{x} \\ (\boldsymbol{w}_i - \boldsymbol{w}_j)^T \boldsymbol{x} &= 0 \end{aligned}$$

Multiclass classification



Multiclass classification

all-pairs

- Learn one binary classifier for each pair of classes:
  - positive examples from one class
  - negative examples from the other
- Predict a new example in the class winning the largest number of pairwise classifications

Generative linear classifiers

Gaussian distributions

- linear decision boundaries are obtained when covariance is shared among classes ($\Sigma_i = \Sigma$)

Naive Bayes classifier

$$
\begin{aligned}
f_i(\boldsymbol{x}) = P(\boldsymbol{x}|y_i)P(y_i) &= \prod_{j=1}^{|\boldsymbol{x}|}\prod_{k=1}^{K}\theta_{ky_i}^{z_k(x[j])}\frac{|\mathcal{D}_i|}{|\mathcal{D}|} \\
&= \prod_{k=1}^{K}\theta_{ky_i}^{N_{k\boldsymbol{x}}}\frac{|\mathcal{D}_i|}{|\mathcal{D}|}
\end{aligned}
$$

- where $N_{k\boldsymbol{x}}$ is the number of times feature k (e.g. a word) appears in $\boldsymbol{x}$

Generative linear classifiers

Naive Bayes classifier (cont)

$$\log f_i(\boldsymbol{x}) = \underbrace{\sum_{k=1}^{K} N_{k\boldsymbol{x}} \log \theta_{ky_i}}_{\boldsymbol{w}^T \boldsymbol{x}'} + \underbrace{\log(\frac{|\mathcal{D}_i|}{|\mathcal{D}|})}_{w_0}$$

- $\boldsymbol{x}' = [N_{1\boldsymbol{x}} \cdots N_{K\boldsymbol{x}}]^T$
- $\boldsymbol{w} = [\log \theta_{1y_i} \cdots \log \theta_{Ky_i}]^T$
- Naive Bayes is a *log-linear* model (as Gaussian distributions with shared Σ)